Coupling High-Energy Ignition with Mechanical Behavior

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To successfully model important National Nuclear Security Administration (NNSA) issues such as high explosives (HE) handling and safety, performance and surety, and survivability to a hostile threat, it is necessary to couple the dynamic mechanical behavior of an explosive with its thermal ignition behavior. We have put forth a promising analysis to accomplish this by using T-Division-developed explosive mechanical models with a thermal ignition model developed in the LANL C-PCS group.

The transition of an unreacted energetic material to a full-up detonated state can be classified into three general categories: 1) shock-to-detonation (SDT), 2) deflagration-to-detonation (DDT), and 3) anomalous-to-detonation (XDT) transition. SDT is the only well-understood process out of the three. SDT is prompt detonation, with typical build-up to detonation times being on the order of a few microseconds. For these short times, the underlying mechanism required to cause a heterogeneous explosive to reach a temperature high enough for a prompt detonation (typically in the range of one to two thousand Kelvin) is energy localization in the form of so-called hotspots. Because the physics of hotspots has been intensely studied, the underlying mechanisms at work in SDT are also believed to be understood. The role of an energetic material's mechanical behavior is believed to be of secondary importance in SDT, although it is known that the amount of damage, contained inclusions, binder concentration, etc., all quantitatively effect SDT to some degree. DDT and XDT are much less well understood, which is unfortunate because these two categories encompass very important NNSA issues: high explosive handling and safety, performance and surety, and survivability to a hostile threat. In DDT and XDT, mechanical properties have a dominating role and will influence the outcome of an initiated chemical reaction—that is, will the reaction extinguish, build up to detonation, or something else in between? Moreover the time for thermal runaway may be very long, say tens of microseconds up to hours. Clearly, to model DDT and XDT there is a need to couple a thermal mechanical model with a thermal ignition model, and that is the focus of the work described here.

To understand the relevant physics that must be captured by a mechanical constitutive theory, imagine a low velocity impact of a high explosive (HE) by a thrown metal fragment. By low velocity, it is meant that the impact is sub-SDT. The HEs of interest in this work are solid heterogeneous explosives, and for LANL the two explosives PBX 9501 and PBX 9502 are preeminent. These are both plastic-bonded explosives, having a high concentration of explosive grains embedded in a polymer-binding matrix. As the incoming fragment collides and penetrates the HE, considerable heating will take place from the mechanical work being done on the explosive at the expense of the fragment's kinetic energy. Adiabatic heating will be one source of temperature rise. This arises from the volumetric compression of the HE ahead of the moving fragment. The compressed HE will heat according to its equation of state (EOS). As the velocity of impact is reduced, inelastic work done on the HE grows in importance. Inelastic heat sources include plastic heating at the process zone of a growing crack in the HE, frictional heating of growing cracks in the presence of a hydrostatic pressure, plastic flow occurring in the explosive grains and the binder, and viscoelastic work done by the polymeric binder. The accumulation of all these heat sources will result in a temperature rise in the impacted explosive. It is this temperature that is fed into the thermal ignition model, and for that the present work invokes the Henson-Smilowitz thermal ignition model.

The Henson-Smilowitz thermal ignition model is physically based and has been parameterized to a wide set of independent explosive initiation experiments. Here we will focus on PBX 9501, which uses octagen (HMX) as its explosive component. Figure 1 shows a schematic of the important decomposition steps in HMX, beginning with the beta-delta solid-solid first-order phase transformation and concluding with a

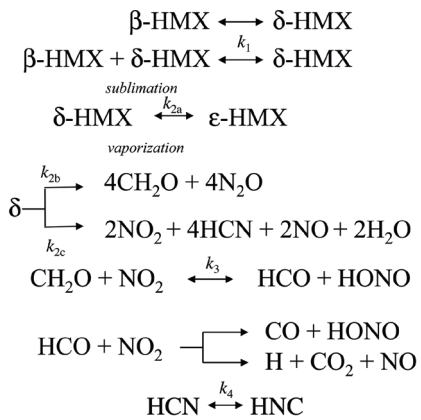

Fig. 1. Schematic of decomposition steps of HMX in the Henson-Smilowitz thermal ignition model.

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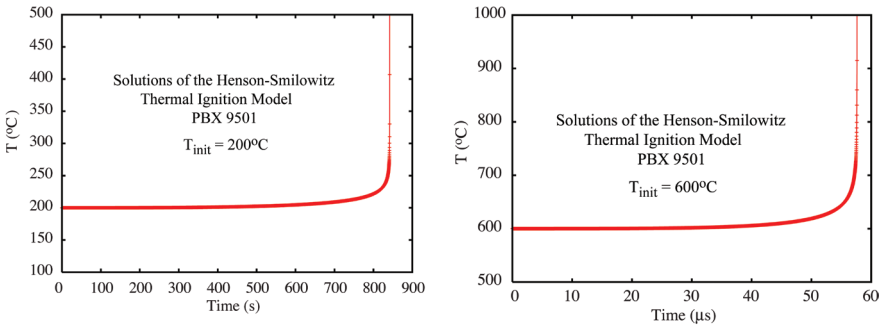

Fig. 2. Solution of the Henson-Smilowitz thermal ignition model for 200ºC (left) and 600ºC (right).

gaseous mixture of decomposition molecules. The Henson-Smilowitz decomposition steps capture the chemistry of both the dark- and bright-zone burning important in HMX decomposition. Each species occurring in Fig. 1 evolves according to a differential equation (DE) for that species concentration in terms of the other decomposition products. Altogether there are six coupled DEs and two DEs describing the temperature and pressure evolution. The coefficients of the DEs are temperature-dependent Arrhenius exponentials, and this is where the temperature from the mechanics described above is first implemented. As the temperature rise from the chemical reaction begins to exceed that from the mechanical work, it is that temperature which is supplied to the Arrhenius exponentials.

Figure 2 is the solution for the Henson-Smilowitz model for two initial temperatures. It is clear that if the mechanical work can exceed 600ºC, then in a low velocity impact lasting 50 to 100 μs, run away behavior is a likely outcome. Finally, Fig. 3 shows the results of a simulation where a thermo-mechanical constitutive model, having all the properties described above, is fully coupled to the Henson-Smilowitz thermal ignition model. In the experiment and the simulation a rectangular steel beam impacts PBX 9501 at a speed of around 100 m/s. The HE simulated temperature near the impactor exceeds 600ºC and chemical reaction has begun, similar to the experiment shown in Fig. 3.

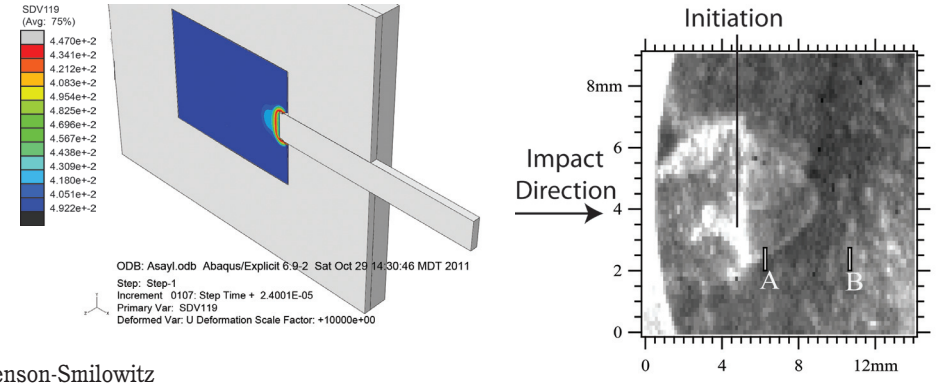

Fig. 3. Temperature profile from a simulation of the impact of PBX 9501 (left), and the corresponding experiment (right). In the left figure, red in the color scheme corresponds to about 600ºC.

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